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Hydromechanical couplings in the clay matrix of argilite: some methodological aspects of the atomistic-to-continuum upscaling

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Context

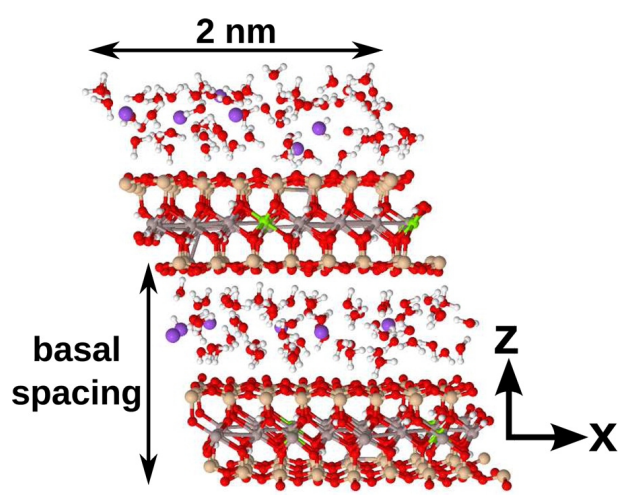
- Clays are ubiquitous in civil engineering applications
- Good knowledge of their mechanical behaviour is necessary
- Swelling clays are highly sensitive to relative humidity
- Hydromechanical couplings *must* be accounted for

$$\sigma = f(\varepsilon, RH)$$

Aim of this study

- Modelling of hydromechanical couplings in the clay matrix of argilite
- Investigation of the influence of local orientational order

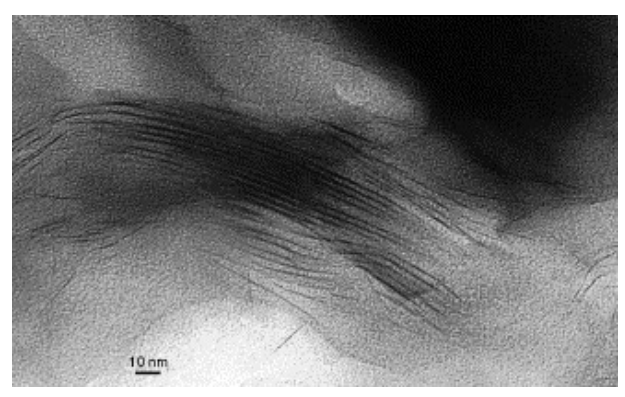
Numerical, multi-scale approach



Microscopic scale : the clay sheet

- Molecular dynamics (μ VT and N Σ T)
- Models developed by Carrier
- Uses theoretical model of Brochard et al. (2012)

Brochard (2012), Jmps 60(4), 606
Carrier (2013), PhD Thesis, Université Paris-Est
Carrier et al. (2014), J. Phys. C 118(17), 8933



Mesoscopic scale : the clay particle

- Rheological models
- Particle viewed as a stack of sheets

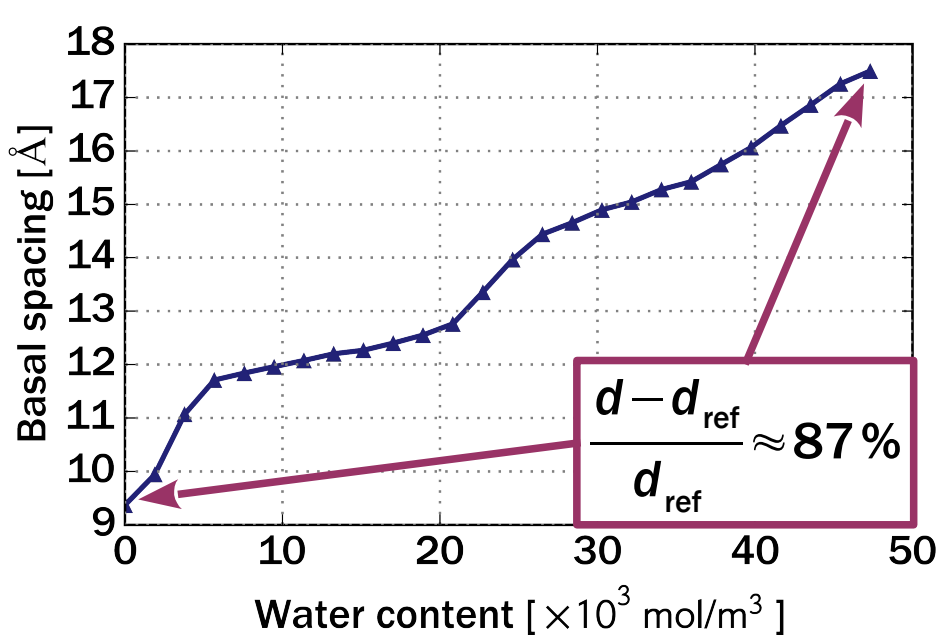


Macroscopic scale : the clay matrix

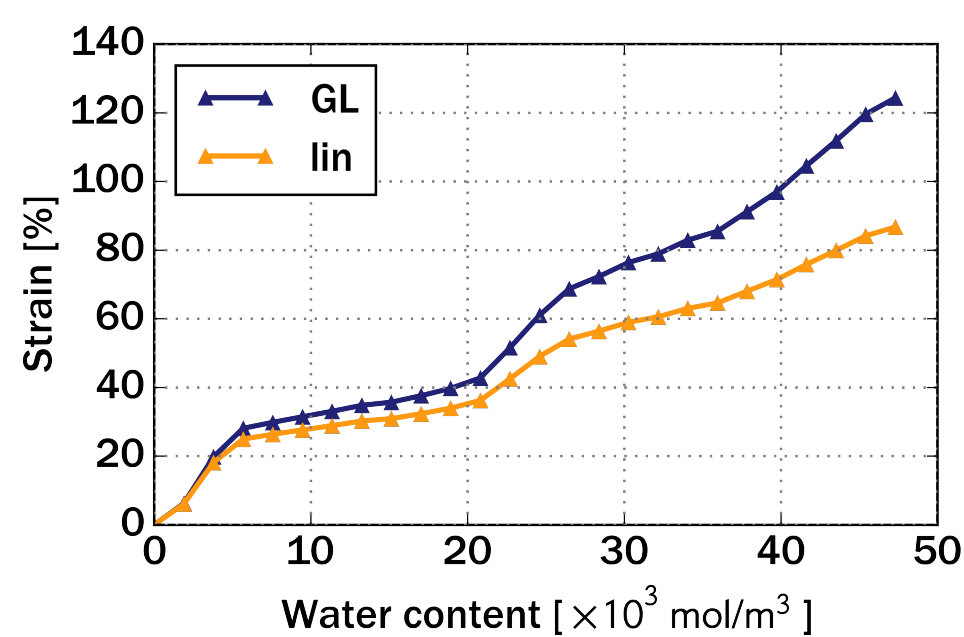
- Viewed as a polycrystal
- FFT-based homogenization methods

Brisard and Dormieux (2010), Comp. Mat. Sci. 49(3), 663
Brisard and Dormieux (2012), CMAME 217-220, 197

Finite strains induced by changes in RH

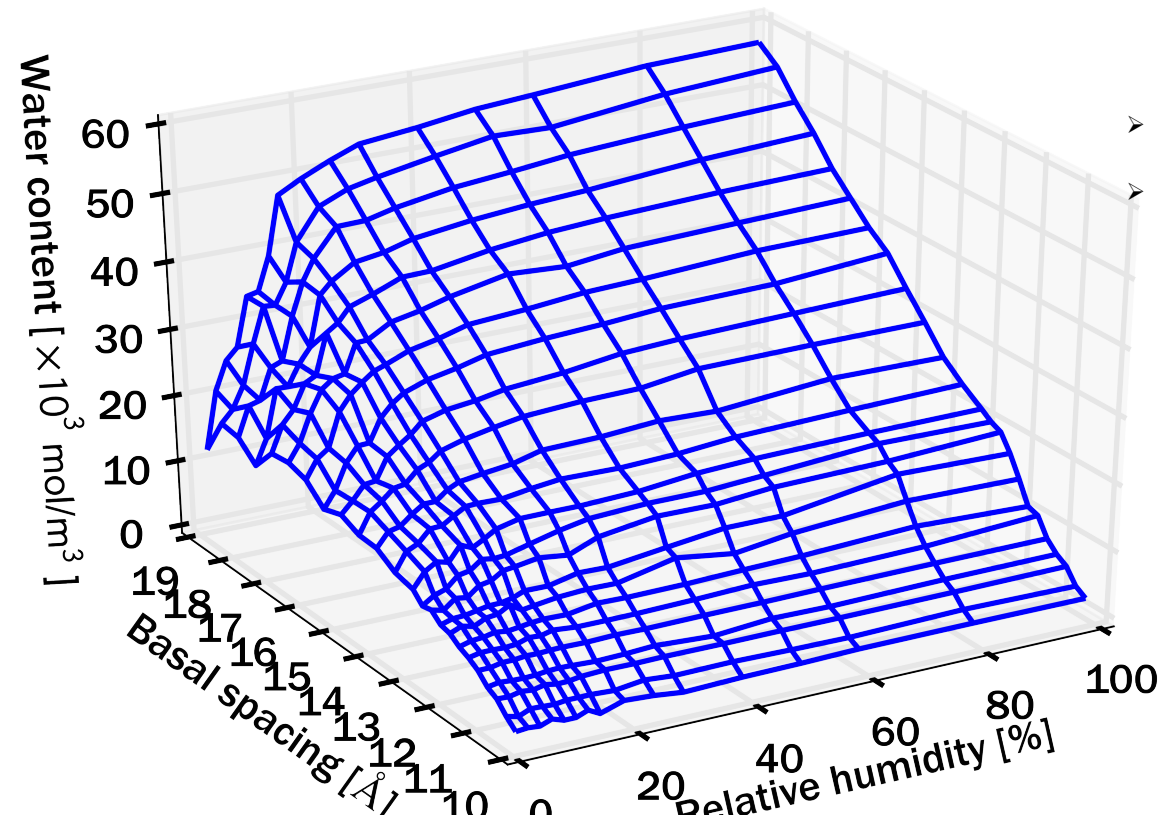


Green-Lagrange strain



$$E = \frac{d - d_{ref}}{d_{ref}} + \frac{1}{2} \left(\frac{d - d_{ref}}{d_{ref}} \right)^2$$

Adsorption isotherms (from B. Carrier, op. cit.)



- Extensive dataset is available
- Derivation w.r.t. RH, d not trivial due to statistical errors: work in progress!

Acknowledgements

This work was financially supported by Défi NEEDS MiPor. We thank: M. Bornert, L. Brochard and E. Ferrage for their advice; E. Ferrage and F. Hubert for their involvement in XRD experiments.

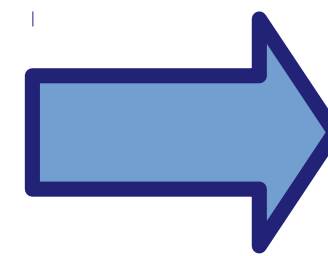
Finite strains formulation of molecular simulations

- How to make sure that molecular simulations return the "right" stiffness?
- Need to understand how N Σ T simulations are run
- Change of geometry of the unit-cell is accepted with probability

$$p \propto \exp \left(- \frac{S(E_{new} - E_{old})}{kT} \right)$$

E_{old} strain in the old configuration (measured)
 E_{new} strain in the new configuration (measured)
 S stress (imposed)

This is an energy change!



- Like in mechanics, S is dual to E.
- The nature of S depends on how we measure E.
- If we measure a GL strain, then S is the Piola II stress.

On the reference configuration

- Strains are measured with respect to a reference configuration
- The stress-free configuration is not unique (depends on the water content)
- Prestressed reference configuration

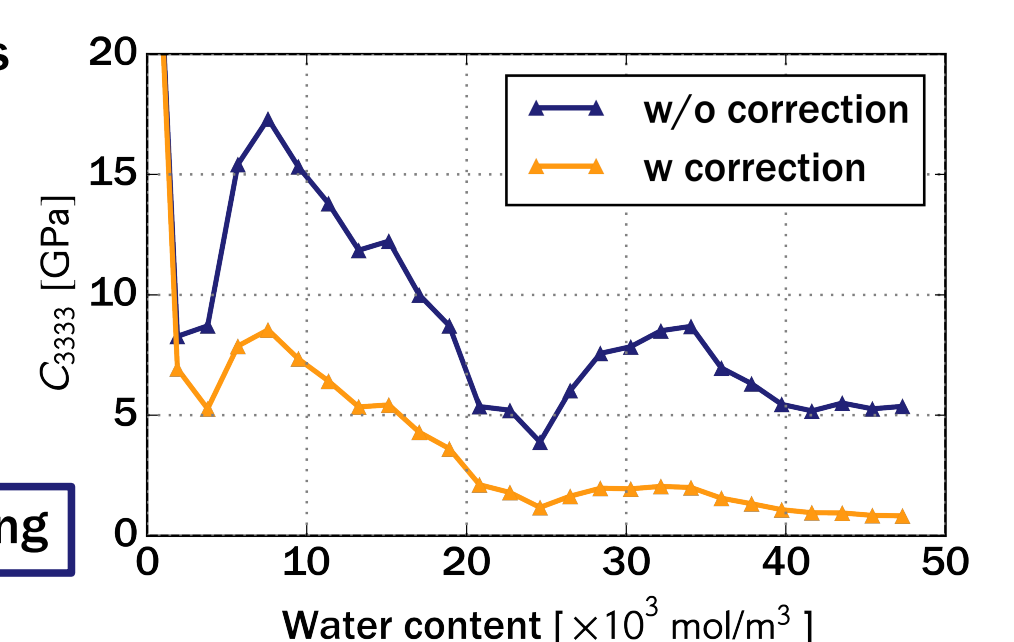
$$S = C_u(n) (E - E_0(n))$$

Free hydric strain
Undrained stiffness

- Correction of molecular dynamics results

$$C_u(n) = \left(\frac{d_{ref}}{d_0(n)} \right)^4 \tilde{C}_u(n)$$

Direct output of MD
Stress-free basal spacing



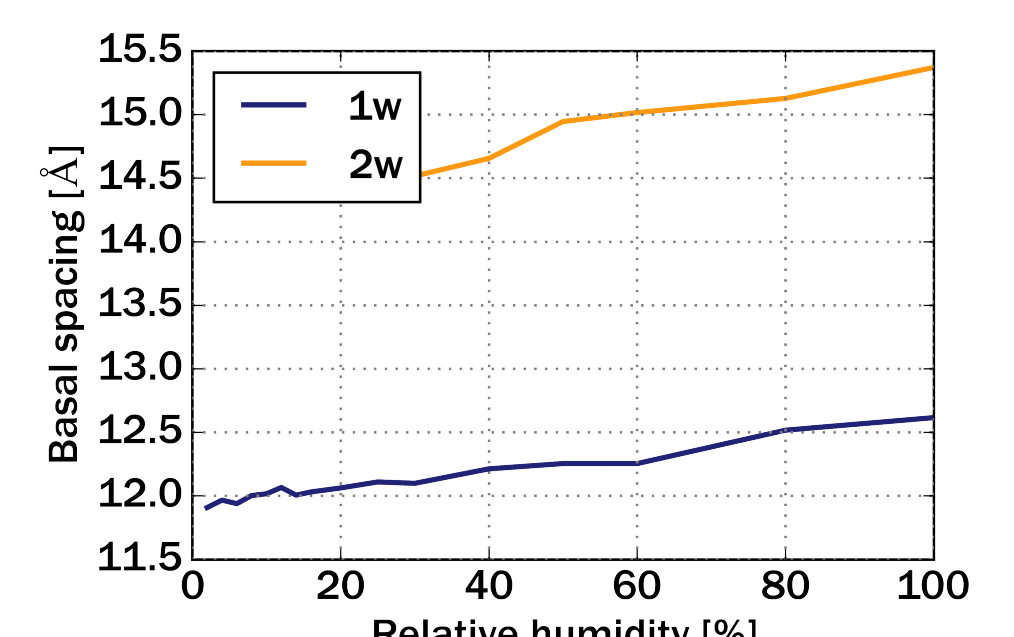
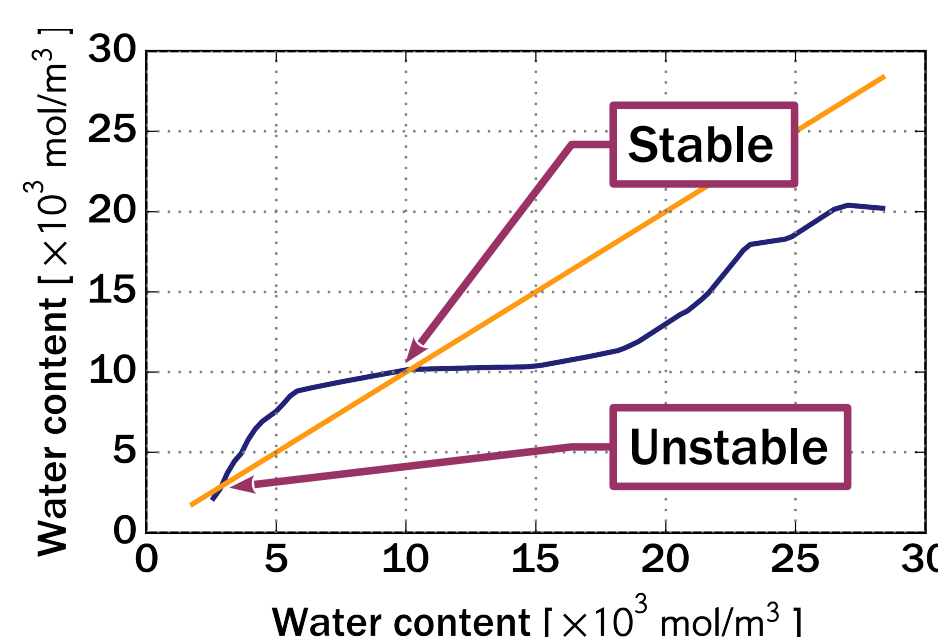
Undrained vs. drained stiffness

- In our MD simulations, the water content is fixed: **undrained** stiffness $C_u(n)$
- In the continuum mechanics simulations (at the scale of the clay matrix), we control the relative humidity (or chemical potential of water): **drained** stiffness $C_d(\mu)$
- We need to perform a change of state variables $(E, n) \rightarrow (E, \mu)$

$$C_d(\mu) = C_u(n) - \left(\frac{\partial n}{\partial \mu} \right)^{-1} \left(\frac{\partial n}{\partial E} \right)^2$$

- Requires the adsorption isotherm $n(d, \mu)$ and its derivatives!

Application: stable equilibria at fixed relative humidity



$$\text{Fixed-point equation } n_{mc}(d_0(n), \mu) = n$$

